Scale up of adsorption experiments

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From big to small or small to big

0.2 mm particles

4 mm diameter pellets

Mathematical model

Model begins by defining and advection-diffusion equation in the void region

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial z}(uc) = D\left[\frac{\partial^2 c}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)\right]$$

$$\phi \pi R^2 \bar{c} = 2\pi \int_0^R cr\, dr$$

Integrating the advection-diffusion equation

$$\frac{\phi R^2}{2}\left[\frac{\partial \bar{c}}{\partial t} + u\frac{\partial \bar{c}}{\partial z}\right] = \frac{\phi R^2 D}{2}\frac{\partial^2 \bar{c}}{\partial z^2} + D\int_0^R \frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) dr$$

$$D\int_0^R \frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) dr = D\sum_j r_j\, c_r|_{r_j}$$

Mathematical model

Equating mass flux at particle boundaries to mass adsorbed within the particles

$$\frac{\partial \bar{c}}{\partial t} + u\frac{\partial \bar{c}}{\partial z} = D\frac{\partial^2 \bar{c}}{\partial z^2} - \frac{(1-\phi)}{\phi}\rho_q\frac{\partial \bar{q}}{\partial t}$$

$$\rho_q = (M_f - M_i)/((1-\phi)AL)$$

Langmuir equation

$$\frac{\partial \bar{q}}{\partial t} = k_a\bar{c}(\bar{q}_m - \bar{q}) - k_d\bar{q}$$

Linearised Langmuir

$$\frac{\partial \bar{q}}{\partial t} = k_l(\bar{q}_e - \bar{q})$$

Dynamic Adsorption Characteristics of Phosphorus Using MBCQ

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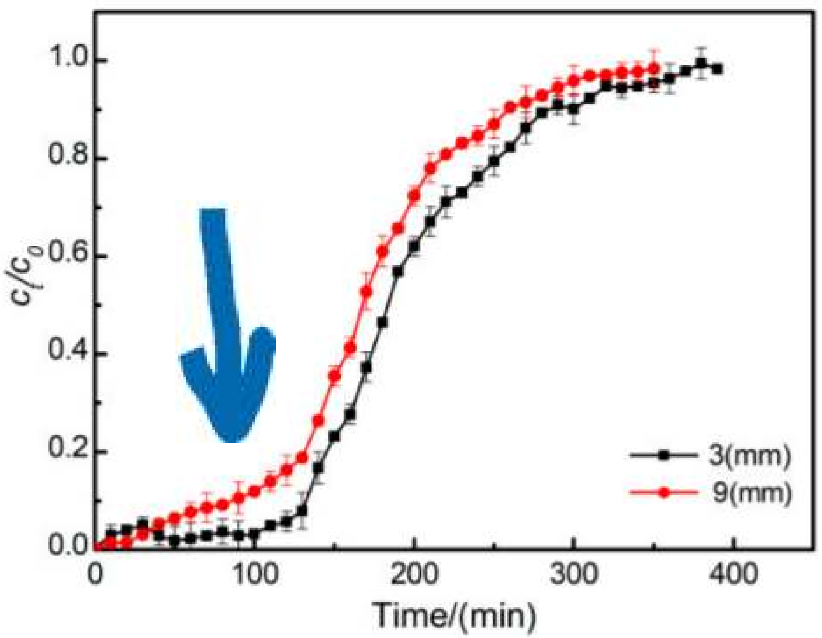


Figure 4. Effects of MBCQ with two particle sizes on the breakthrough curves.

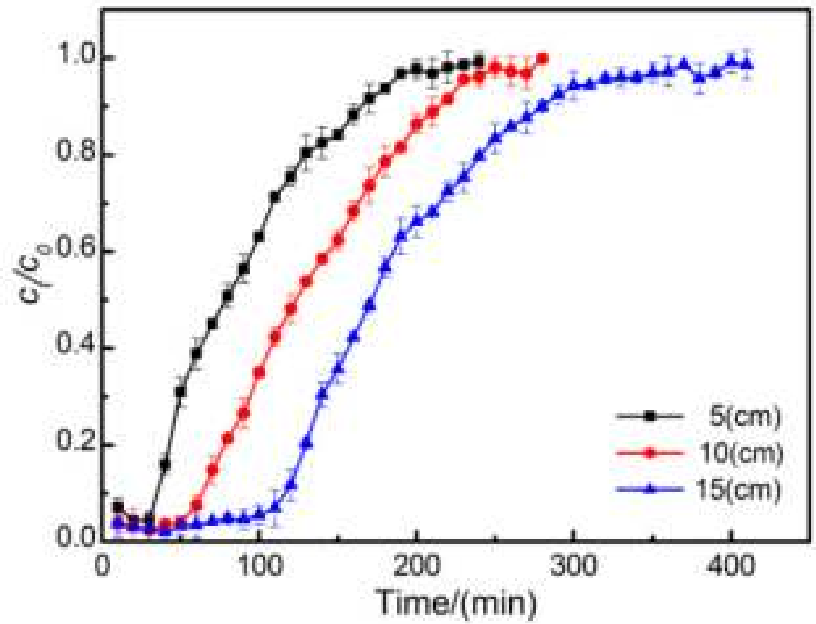


Figure 7. Effects of bed height on breakthrough curves.

Model 1

$$Da\frac{\partial \bar{c}}{\partial t} + \frac{\partial \bar{c}}{\partial z} = Pe^{-1}\frac{\partial^2 \bar{c}}{\partial z^2} - \frac{\partial \bar{q}}{\partial t}$$

$$\frac{\partial \bar{q}}{\partial t} = 1 - \bar{q}\,,$$

Advection-diffusion model with linear Langmuir

$$\mathcal{L} = uc_{in}\tau\phi/((1-\phi)\rho_q q_e) \qquad \tau = 1/k_l$$

Length and time scales

Model 1: Travelling wave solution

$$Da\frac{\partial \bar{c}}{\partial t} + \frac{\partial \bar{c}}{\partial z} = Pe^{-1}\frac{\partial^2 \bar{c}}{\partial z^2} - \frac{\partial \bar{q}}{\partial t}\,.$$

$$\frac{\partial \bar{q}}{\partial t} = 1 - \bar{q}\,,$$

Define $\eta = z - s(t)$ where $s_t = v$ and $\bar{c}(z,t) = C(\eta)$, $\bar{q}(z,t) = Q(\eta)$

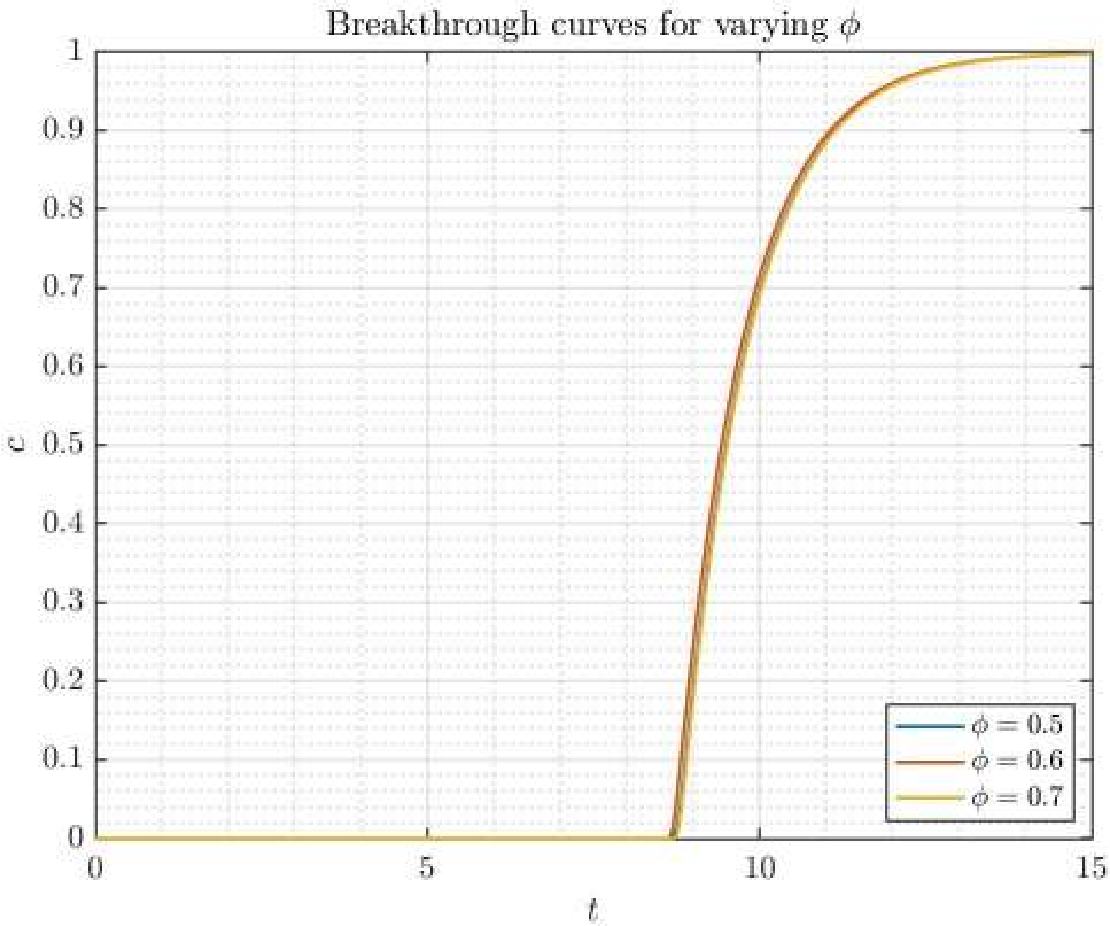
$$-vDa\frac{\partial C}{\partial \eta} + \frac{\partial C}{\partial \eta} = Pe^{-1}\frac{\partial^2 C}{\partial \eta^2} + v\frac{\partial Q}{\partial \eta}$$

$$C(0) = C_\eta(0) = 0 \quad Q(0) = 0$$

$$-v\frac{\partial Q}{\partial \eta} = 1 - Q\,,$$

Travelling wave solution

Phi has no effect



Model 2

$$Da\frac{\partial \bar{c}}{\partial t} + \frac{\partial \bar{c}}{\partial z} = Pe^{-1}\frac{\partial^2 \bar{c}}{\partial z^2} - \frac{\partial \bar{q}}{\partial t}\,.$$

$$\frac{\partial \bar{q}}{\partial t} = \bar{c}(1-\bar{q}) - \frac{k_d}{k_a c_{in}}\bar{q}\,.$$

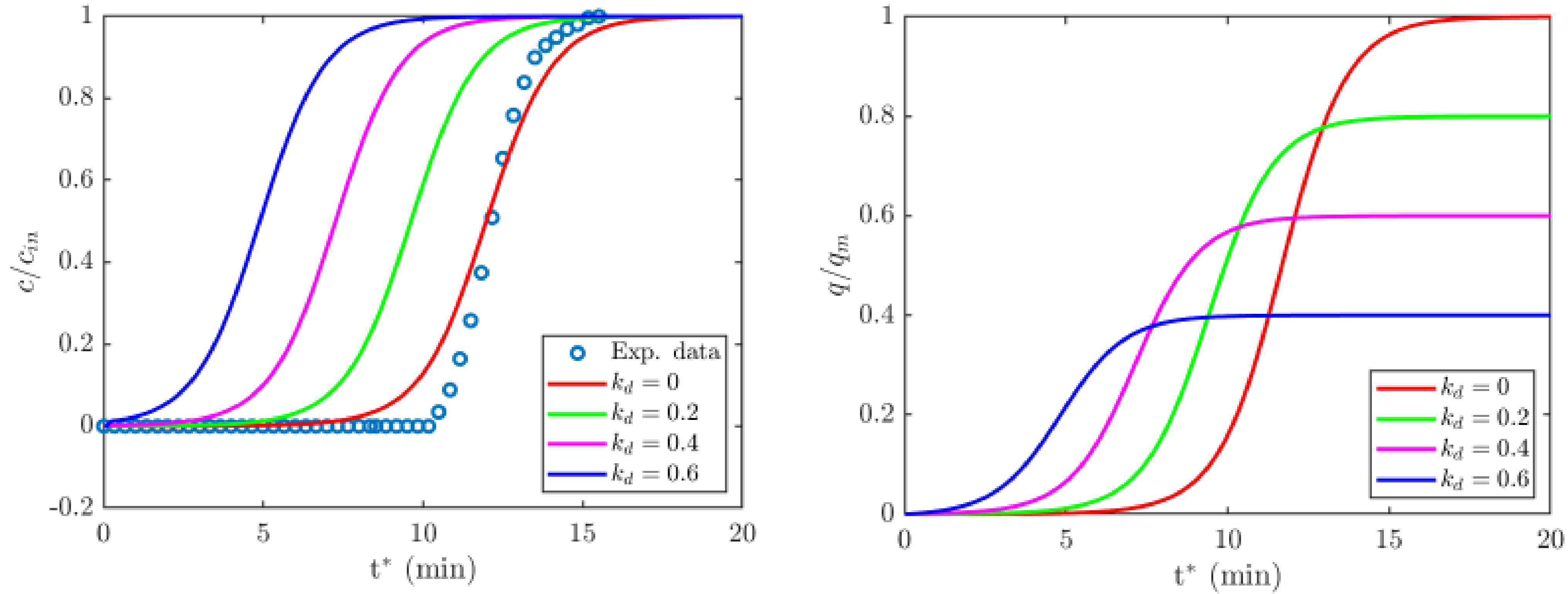
Advection-diffusion model with full Langmuir

$$\mathcal{L} = u c_{in} \tau \phi / ((1-\phi)\rho_q q_e)$$

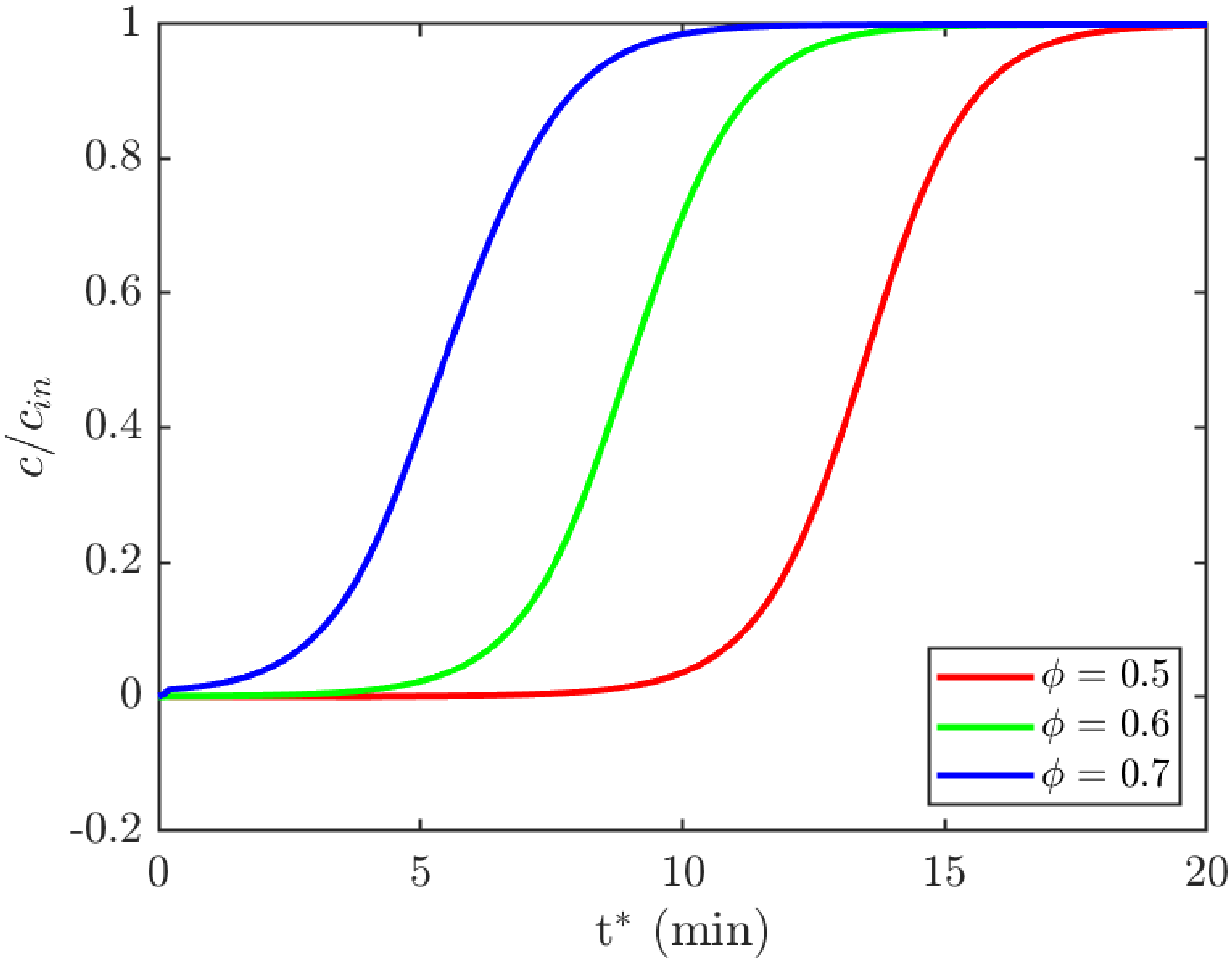
$$\tau = 1/(k_a c_{in})$$

Length and time scales

Full Langmuir equation



Increasing kd doesn't affect form of breakthrough, but does affect time. Large effect on equilibrium q



Fixed kd=0.1

Again, changing phi makes no difference to the solution form

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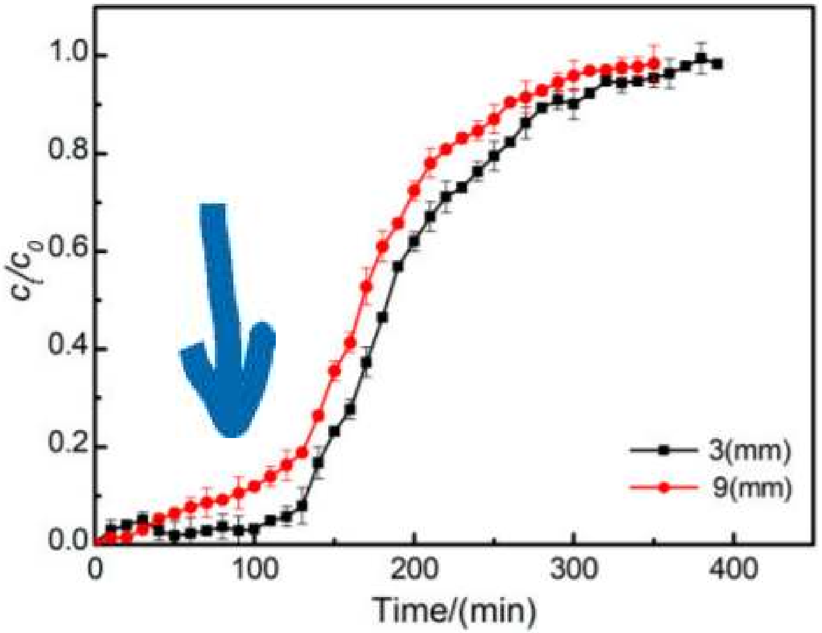


Figure 4. Effects of MBCQ with two particle sizes on the breakthrough curves.

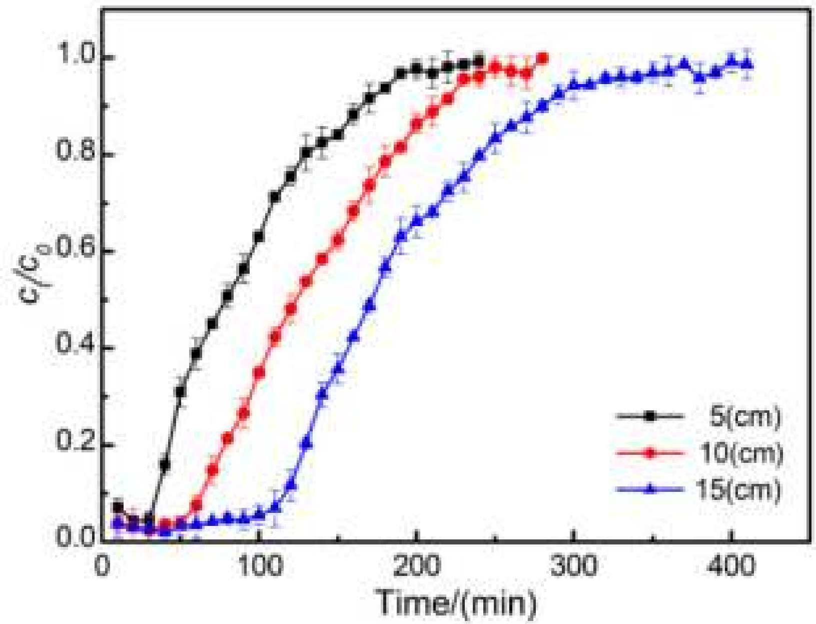


Figure 7. Effects of bed height on breakthrough curves.

Initial breakthrough suggests different mechanism ..

Assume contaminant flows through void region and then diffuses into the particle and finally is adsorbed inside the particle

Consider a cylindrical cross-section particle

$$\phi_p \frac{\partial c_p}{\partial t} = \phi_p \frac{D_p}{r_p} \frac{\partial}{\partial r_p} \left(r_p \frac{\partial c_p}{\partial r_p} \right) - (1 - \phi_p) \rho_q \frac{\partial q}{\partial t}$$

$$D_p \frac{\partial c_p}{\partial r_p} = D \frac{\partial c}{\partial r} \qquad \left(D_p \frac{\partial c_p}{\partial r_p} = k_f (\bar{c} - c_p) \right) \bigg|_{r_p = a_p}$$

Recall the final integral

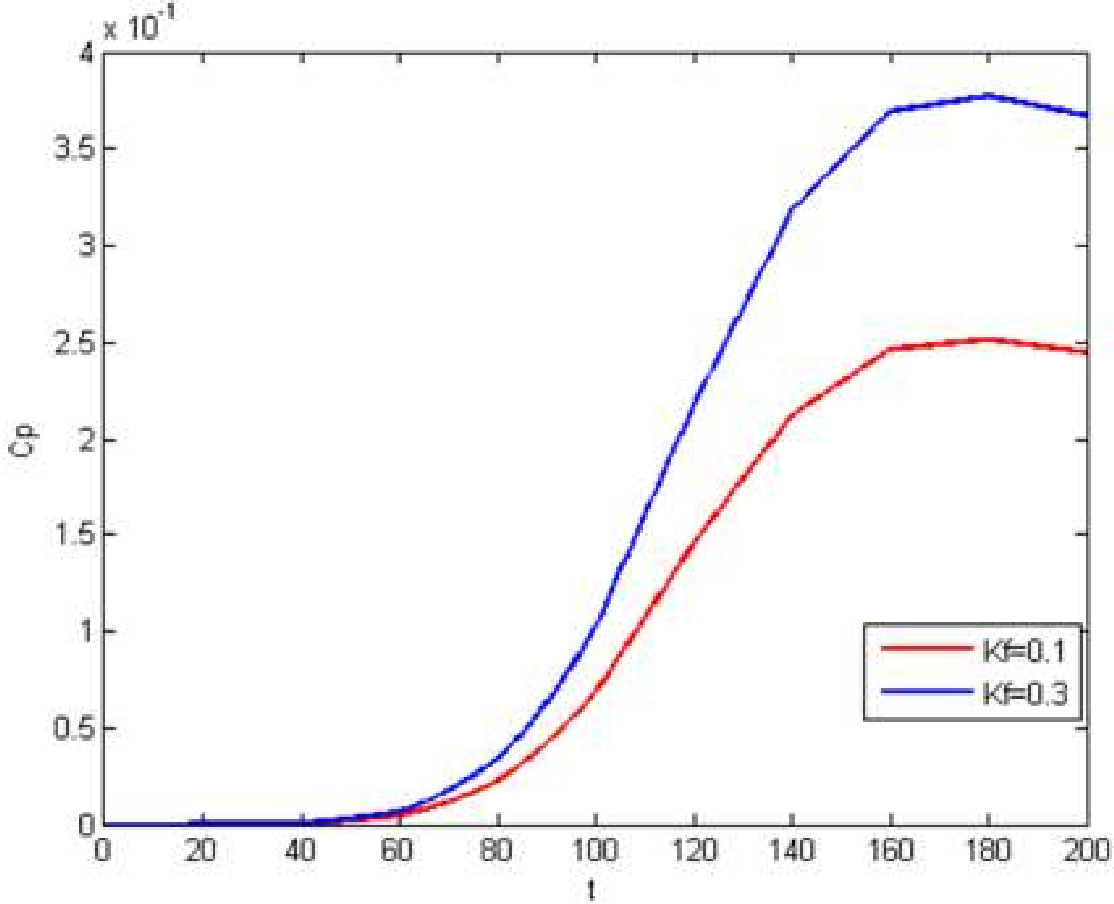
$$D\int_0^R \frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)dr = D\sum_j r_j\, c_r\big|_{r_j} = D_p\sum_j r_j\, c_{pr}\big|_{r_j} = k_p(\bar{c} - c_p\big|_{a_p})\sum_j r_j$$

define $\sum r_j = \xi$ as the shape factor

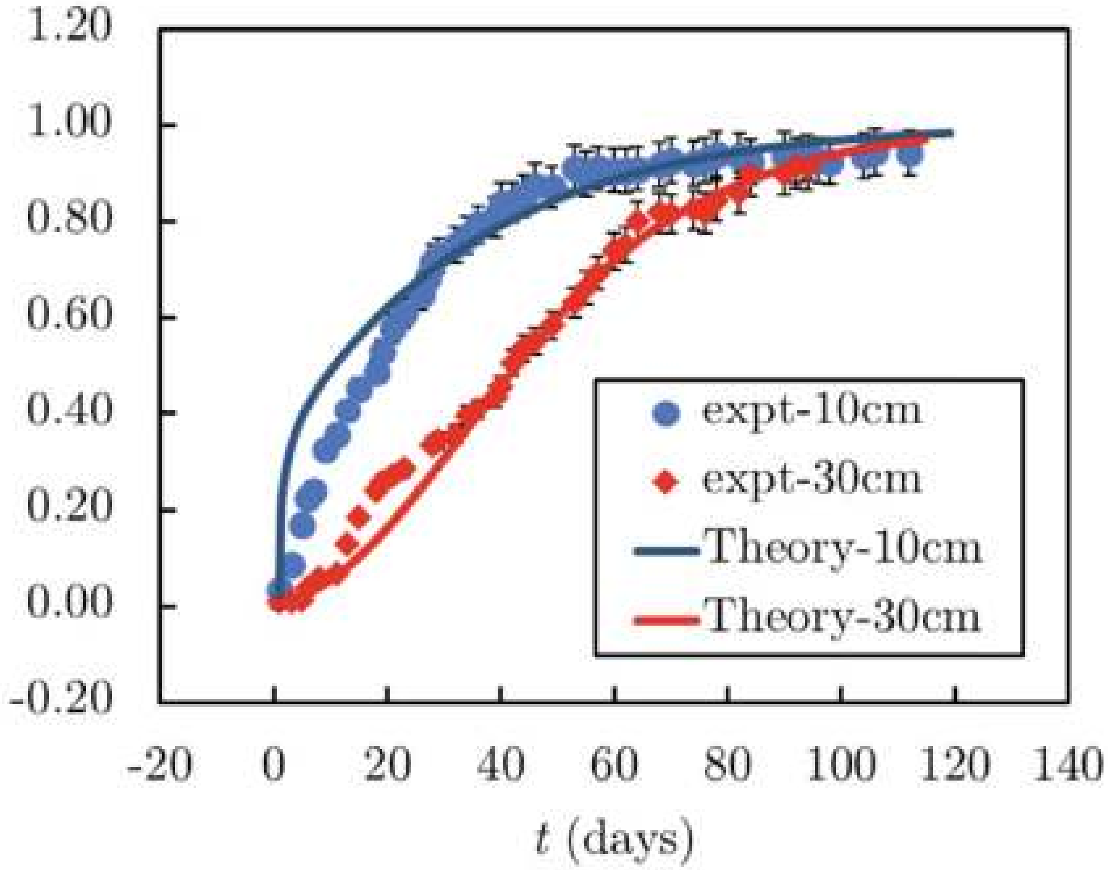
$$\frac{\partial \bar{c}}{\partial t} + u\frac{\partial \bar{c}}{\partial z} = D\frac{\partial^2 \bar{c}}{\partial z^2} - \frac{2\xi k_f}{\phi R^2}(\bar{c} - c_p\big|_{r_p=a_p})$$

$$\frac{\partial \bar{q}}{\partial t} = k_a c_p(\bar{q}_m - \bar{q}) - k_d\bar{q}$$

Leaving a coupled system of advection-diffusion, diffusion in a particle and Langmuir


x 10^-1
4
3.5
3
2.5
2
1.5
1
0.5
0
Cp
0
20
40
60
80
100
120
140
160
180
200
t
Kf=0.1
Kf=0.3

- Awaiting results but … this form has different time-scales: flow, diffusion and adsorption suggesting more complex behaviour. Seems the best option.



Taken from Mondal et al, Chem. Engng Sci. 2019

To do

- We can capture a given data set but the obtained parameter values will not provide the correct solution form for larger particles
- Finish the particle diffusion model and investigate appropriate parameter regimes. This seems a promising route and should allow scale up.
- Find more data to verify models

- Alba – experiments with same components but different size columns